

A PHASE-FIELD THEORY OF DISLOCATIONS: STATISTICAL MODELING OF PLASTICITY AND NETWORKS IN GRAIN BOUNDARIES

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A phase-field theory of dislocations, strain hardening and hysteresis in ductile single crystals is developed. The theory accounts for an arbitrary number and arrangement of dislocation lines over a slip plane; the long-range elastic interactions between dislocation lines; the core structure of the dislocations; the interaction between the dislocations and an applied resolved shear stress field; and the irreversible interactions with short-range obstacles, resulting in hardening, path dependency and hysteresis.

We introduce a variational formulation for the statistical mechanics of dissipative systems. The influence of finite temperature as well as the mechanics in the phase-field theory is modeled with a Metropolis Monte Carlo algorithm and a mean field approximation.

A chief advantage of the present theory is that at zero temperature it is analytically tractable, in the sense that the complexity of the calculations may be reduced, with the aid of closed form analytical solutions, to the determination of the value of the phase field at point-obstacle sites.

The theory predicts a range of behaviors which are in qualitative agreement with observation, including hardening and dislocation multiplication in single slip under monotonic loading; the Bauschinger effect under reverse loading; the fading memory effect; the evolution of the dislocation density under cycling loading; temperature softening; strain rate dependence; and others.

The model also reproduces the formation of dislocation networks observed in grain boundaries for different crystal structures and orientations. Simultaneously with the stable configurations the theory naturally predicts the equilibrium dislocation density independently of initial values or sources.